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CEWES MSRC / PET TR / 98-06

Contract Year Two Programming Environment and Training (PET) Additional Focused Efforts for CEWES Major Shared Resource Center (MSRC)

5 February 1998

Prepared For:
CEWES MSRC
U.S. Army Corps of Engineers
Waterways Experiment Station (CEWES)
Vicksburg, MS

02h00898

BACKGROUND

As a result of the Mid-Year Review for the U.S. Army Corps of Engineers Waterways Experiment Station (CEWES) Major Shared Resource Center (MSRC) Programming Environment and Training (PET) program that occurred on 22-23 September 1997, additional Focused Efforts were approved for the primary Computational Technology Areas (CTAs) supported by the center and for other specialty areas.

NEW FOCUSED EFFORTS

The following additional Focused Efforts have been approved for Year Two:

Mississippi State University - ERC

ï Message Passing Interface (MPI) Support for SPP Algorithm Migration -- expanded to include installation of MPICH on the T3E

ï Terascale Vis -- Visualization of Large Datasets at CEWES MSRC

CRPC - Rice/Tennessee/Syracuse

ï Interoperable CTA Software Repositories (Tennessee)

ï MPI Interconnection and Process Management (Tennessee)

ï Tango for Collaboration and Distance Consulting (Syracuse)

ï Parallel CMS Planning (Syracuse)

ï HPCC Educational CD-ROM (Syracuse)

ï Object Web RTI Prototype (Syracuse)

TICAM - University of Texas

ï 3-D ADCIRC Parallel Migration

ï Incorporation of PARSim into GMS

Detailed descriptions of these Focused Efforts are provided in Appendix A.

Appendix A: Detailed Focused Effort Descriptions

1. Title: Message Passing Interface (MPI) Support for SPP Algorithm Migration --
expanded to include installation of MPICH on the T3E

Thematic Area(s): Scalable Computing Migration

PI Name: Dr. Anthony Skjellum (MSU-ERC)

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Project Description: MPICH will be ported to the T3E at CEWES MSRC.

Benefits: The present Cray version of MPI on the T3E is not adequate to meet the
needs of the CEWES MSRC users in migrating codes onto this machine.
The availability of MPICH on the T3E will greatly facilitate this migration
in support of MSRC users in general, CHSSI projects, and DoD Challenge
Projects. This is also in direct support of the CEWES MSRC hardware
acquisition strategy to move away from large vector processors toward
scalable parallel processors.

Deliverables: MPICH on T3E

Notes: Porting and installation will require five months, followed by several
months of lower-level activity in maintenance.

Customer Commitment/Involvement: MPICH on T3E has been requested by CEWES
MSRC users.

2. Title: Terascale Vis -- Visualization of Large Datasets at CEWES MSRC

Thematic Area(s): SciVis for Very Large Problems

PI Name: Dr. Raghu Machiraju (MSU-ERC)

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Project Description: Computational field simulations of large-scale physical phenomenon produce data of unprecedented size (terabytes), which introduces new challenges to the management and visual analysis of data. A system which facilitates the visual analysis of data will be concerned with the storage, representation, access and interpretation of data. Visual computing researchers at national laboratories [1], universities and commercial companies have begun to address this problem, which seeks solutions [2] from a variety of areas including compression techniques, database access, high performance computing and user interaction techniques. The three-fold goals of this effort are:

ï   Examine the visualization needs of CEWES MSRC users with terascale datasets
ï   Survey of current methods for terascale visualization
ï   Propose solutions using existing technology and/or new techniques

Visits to selected sites of active research in terascale visualization will be made for purposes of increasing awareness and exploring collaboration opportunities.

Benefits: The benefits of an in-depth study include:

ï   Definition of this problem from a CEWES MSRC perspective
ï   Clarification of the issues involved
ï   Development of local expertise in terascale visualization at CEWES MSRC
ï   Development of a long-range plan for local solutions

Specifically, the survey will cover aspects of:

ï   Feature detection (including wavelets) -- identification of significant regions
ï   Compressed multi-resolution representations of grids (structured, unstructured)
ï   Interactive exploratory techniques in multiple resolutions
ï   Image based techniques, including IBR (image based rendering)

- ï Database access and search based on image and text queries
- ï Human-centric and perceptual considerations
- ï Systems and performance issues (e.g., out-of-core techniques, parallel processing)
- ï Approach from a data-mining perspective

Deliverables: A report on the state-of-the-art in terascale visualization and a plan for the future from the CEWES MSRC perspective.

Customer Commitment/Involvement: Has been requested by CEWES MSRC users. Users in CFD, CSM, CWO, EQM will participate in evaluation.

References:

[1] Terascale Visualization: Approaches, Pitfalls, and Issues Panel, C. Hunter, R. Crawfis (Chairs), Visualization '97 Conference.

[2] Visualizing Large Data, Birds of a Feather Session, Kwan-Liu Ma (Organizer), Visualization '97 Conference.

3. Title: Interoperable CTA Software Repositories

Thematic Area(s): HPC Training and DoD User Productivity

PI Name: Dr. Shirley Browne (UTenn)

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PI Telephone: (423) 974-8295   **PI Fax:**   (423) 974-8296

Project Description: The DoD HPCMP effort will undoubtedly produce an abundance of software and other reusable assets. A system is needed whereby these assets can be archived and shared among the MSRCs, DCs, and other DoD sites and users. One system that can meet this need is the Repository in a Box (RIB) toolkit developed by the University of Tennessee. Tennessee proposes to apply RIB, with necessary extensions of its functionality, to set up a distributed collection of interoperable software repositories for the DoD HPCMP CTAs. This network of repositories will allow codes, algorithms, and experiences to be shared within and between CTAs. Use of RIB will provide a uniform and consistent user interface to these repositories.

With ASC MSRC and ARL MSRC funding, Tennessee is initially setting up interoperable software repositories for CCM (ASC and ARL), CEN (ASC), and SIP (ARL). These repositories are being set up using the NHSE RIB toolkit which uses an IEEE software cataloging standard that enables interoperation (e.g., exchange of software catalog records) between repositories. The interoperation capability allows sharing within and among MSRCs and CTAs. With CEWES MSRC funding, Tennessee will set up an additional repository for the CFD CTA. CFD is an excellent candidate for an interoperability experiment, since it is supported at all four MSRCs. CEWES MSRC will take the lead in coordinating with the CFD leads at the other sites to agree on a common classification scheme, and then each site would catalog software in its specialty sub-areas of CFD and import each other's records to give its users a view of the entire distributed set of CFD software. University of Tennessee staff will work with the CEWES MSRC Webmaster to set up RIB at CEWES MSRC and will assist CFD leads in using RIB.

Benefits: Software repositories support the Common HPC Software Support Initiative (CHSSI) by providing a means to disseminate codes that have been developed. Multi-architecture portability is encouraged by having software quality control guidelines that stress portability. The availability of efficient well-tuned parallel codes will improve effective utilization of HPC resources.

Deliverables:

> Oct 97
> Determine appropriate interoperation architecture and access control requirements
>
> Oct-Dec 97
> Extend RIB functionality
> Work with domain experts in CFD on customizing the data model, classification hierarchy, and quality control guidelines, and on identifying candidate software
>
> Nov 97
> Repository interoperability demonstration at SC97
>
> Jan 98
> Install and test new version of RIB
>
> Jan-Mar 98
> Implement pilot CTA repositories and discussion lists

Customer Commitment/Involvement: The CFD, CEN, and EQM CTA white papers requested mechanisms for code, algorithm, and experience sharing. Dr. Steve Bova, the on-site CFD lead at CEWES MSRC, and Dr. Ehtesham Hayder, who has expertise in the CFD area, have agreed to help with this project at CEWES MSRC.

4. Title: MPI Interconnection and Process Management

Thematic Area(s): Scalable Computing Migration, HPC Performance Metrics/Tools, DoD Challenge Applications

PI Name: Dr. Jack Dongarra (UTenn)

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Project Description: Currently, different vendor MPI implementations cannot interoperate directly with one another. As a result, use of distributed computing across different vendor platforms requires use of a single MPI implementation, such as MPICH. This solution may be sub-optimal, because it cannot utilize the vendors' own optimized MPI implementations. PVMPI, a software package currently under development at the University of Tennessee, provides the needed interoperability among different vendors' optimized MPI implementations. As the name suggests, PVMPI is a powerful combination of the proven and widely ported Parallel Virtual Machine (PVM) system and MPI. PVMPI is transparent to MPI applications and allows intercommunication between different MPI implementations (or instances of the same implementation) using normal MPI communication calls. Additionally, PVMPI allows flexible control over MPI applications by providing access to all the process control and resource control functions available in the PVM virtual machine. For more information about PVMPI, see http://www.netlib.org/mpi/pvmpi/pvmpi.html.

The main goal of the PVMPI project is to allow different MPP vendor MPI implementations to inter-communicate to allow the use of multiple MPPs in solving challenging problems. Intercommunication allows users to place each section of an application on the system most suited for its execution. Targeted users of PVMPI are those who have such multi-platform applications and those who need dynamic process control and cannot wait for MPI-2 to appear. For CEWES MSRC, Tennessee proposes to identify Forces Modeling and Simulation (FMS) and other application areas that require these capabilities and apply the PVMPI system to provide them.

Benefits: MPI intercommunication will improve the effective utilization of HPC resources by allowing each section of a complex application to be placed on the system most suited for its execution.

Several CTAs have expressed a need for MPI dynamic process management and intercommunication. The FMS CTA in particular has a

8

need for interoperation between different MPI implementations because of the distributed nature of FMS applications. Applications in all CTAs that require the use of multiple platforms (e.g., computation on an MPP coupled with visualization on a visualization engine) will benefit from intercommunication capabilities.

Deliverables:

Oct 97
Identify candidate applications needing MPI dynamic process control and intercommunication capabilities and select a small number for implementation of these capabilities

Oct-Dec 97
Port PVMPI to additional platforms (T3E, O2K). Implement any additional functionality required by applications.

Jan-Mar 98
Demonstrate MPI dynamic process control and intercommunication on selected FMS and possibly other applications.

Customer Commitment/Involvement: The need for MPI dynamic process control and intercommunication was discussed at the 22-23 Sep 97 CEWES MSRC PET Mid-Year Review.

5. Title: Tango for Collaboration and Distance Consulting

Thematic Area(s): HPC Training and DoD User Productivity

PI Name: Dr. David Bernholdt (NPAC-Syracuse)

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Project Description: The Tango collaboration system has been used successfully in another CEWES MSRC PET Focused Effort to support collaboration in the form of remote classroom instruction, demonstrating the utility of such a system for use within the DoD. This proposal seeks to further extend the application of the Tango collaborative framework to another area of great importance to the DoD and the PET program: technical collaboration among geographically distributed groups, especially in the area of HPCC software development and consulting (i.e. PET or MSRC staff working with remote HPCC users).

Tango already includes basic collaborative tools, such as audio/video conferencing, shared whiteboard, chat tool, etc. This project will augment the system with tools necessary to support software development, performance improvement, and related activities.

Early work will include detailed training in the operation and maintenance of the Tango server for appropriate CEWES MSRC staff and installation of the basic Tango system (including server) at CEWES MSRC, making it available to MSRC users for basic collaboration. Development of the additional tools will be done in cooperation with an appropriate group (to be identified), and at the end of the project, the entire system will be available for general use.

Benefits: This project represents a further step in trying to reduce the "importance of place" in access to MSRC resources and MSRC and PET services, as well as in DoD research efforts as a whole.

Deliverables:
- ï Tango server will be deployed on a suitable host at CEWES MSRC
- ï Training in the operation and maintenance of the Tango server will be provided at Syracuse University
- ï Training at CEWES MSRC to familiarize users with the operation and use of the Tango system.
- ï Enhancements to Tango suitable for collaborative software development and consulting, including

- Shared source code viewer/modifier: Syracuse will develop a collaborative version of emacs, a public domain editor with very strong support for code developers. NPAC will provide extensions for collaborative viewing/editing and extend support for a versioning to synchronous collaborative mode. Emacs support for the basic development cycle (code -- compile -- execute -- debug) will be extended to the collaborative mode so that all these steps can be shared by all team members.
- Shared flow diagramming tool: Syracuse will extend functionality of our shared whiteboards to a fully object-oriented, editable, shared drawing tool. This tool will enable users to work on graphical representations of their computational processes, such as flow diagrams and entity relationships models. Shared debugger: NPAC will implement a tool allowing for distribution of the results of a code debugger, either real-time or post-mortem.
- Shared numerical results visualizer: Syracuse will provide the infrastructure supporting shared, distributed, real-time visualization of the numerical results produced by codes running on HPCC platforms. The framework will consist of a runtime for transparent, distributed visualization and of the application programmer interface allowing for an easy hookup of the codes to the visualization system. The runtime will provide a reach set of numerical filters and the store-and-animate capability for analyzing code numerical stability or for tracing numerical convergence processes. A prototype of such a tool has been already implemented at NPAC. Written entirely in Java, the framework is extremely portable and easy to use.
- Java MPI performance visualization: Syracuse will study the feasibility of building a sharable, distributed interface to the tools providing basic performance metrics of HPCC platforms. NPAC will select the most promising performance visualization packages from among public domain systems such as AIMS from NASA or Pablo from University of Illinois, or commercial systems such as Datametrix, IBM perfmon, or SGI Co-Pilot.

Customer Commitment/Involvement: CEWES MSRC has already expressed a desire for a full-scale Tango installation (including server), and for training in the care and feeding of such a system. This project also requires a group willing to help with the design and testing of the new remote consulting/software development tools for Tango, but there are many candidates and we do not anticipate problems identifying a suitable candidate.

6. Title: Parallel CMS Planning

Thematic Area(s): Scalable Computing Migration

PI Name: Dr. David Bernholdt (NPAC-Syracuse)

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Project Description: The Comprehensive Mine Simulator (CMS) is an important FMS application which currently runs on (uniprocessor) SGI systems. Currently the system can handle 30,000-50,000 mines on a single host, but has a target of 1,000,000 mines, which clearly cannot be achieved without migrating to HPC systems.

This project will enable an examination of the application and working with the code developers in order to understand the detailed requirements and effort required to parallelize this application. This will allow NPAC to reliably scope and plan for the actual parallelization, which would be a follow-on project. NPAC will work with Steve Bishop's group at the Night Vision Directorate, Ft. Belvoir, VA to define a reasonable collaborative approach to the actual parallelization effort.

Benefits: This project was recommended by the FMS CTA lead to increase the usability of HPC systems by FMS researchers.

Deliverables: Report and Project Proposal for CMS parallelization effort (March 1998)

Customer Commitment/Involvement: Based on information provided by the FMS CTA lead, NPAC plans to work with Steve Bishop, Night Vision Directorate, Ft. Belvoir, VA and anticipate that the follow-on parallelization project will be a joint effort.

7. Title: HPCC Educational CD-ROM

Thematic Area(s): HPC Training and DoD User Productivity

PI Name: Dr. David Bernholdt (NPAC-Syracuse)

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Project Description: NPAC and other PET partners have a sizable volume of educational materials on various areas of HPCC which are suitable for asynchronous use, for example by DoD researchers wishing to increase their familiarity with various HPCC techniques and tools through self-study. The idea behind this project is to collect such materials into a CD-ROM which can then be distributed to users.

NPAC already has the core of such a collection in a CD-ROM that was produced for Computational Science Education work in China (http://www.npac.syr.edu/projects/pcrc/cpswt-e/). NPAC will remove web technologies (except for Java for computational science) and include Virtual Programming Laboratory and SciVis material. NPAC will then augment this with additional materials (i.e. grids, algebra, programming tools) drawn from other PET partners, guided by an editorial board including (NPAC suggests) Jack Dongarra, Geoffrey Fox, Chuck Koelbel, Joe Thompson, and Louis Turcotte.

NPAC envisions this as an on-going project, with regular releases of new CDs containing updated materials in order to keep abreast of evolving tools and technologies. The current proposal includes funds for NPAC to update materials, coordinate the acquisition of additional materials, and produce the first CD distribution. It also includes funds to support other contributors updating and formatting their materials appropriately for this method of dissemination. As a practical matter, NPAC expects these funds to go directly from NRC to the appropriate universities, thus avoiding additional costs and delays.

Benefits: This project is intended to provide a broad range of HPCC educational material to DoD researchers to augment the more specific training classes available at the MSRCs. It will help researchers make better use of the HPCC resources, and help them better understand which training can be most helpful to them.

Deliverables: CD-ROM produced and ready for distribution (March 1998)

Customer Commitment/Involvement: This project was specifically requested by Louis Turcotte to augment the training initiatives of CEWES MSRC.

8. Title: Object Web RTI Prototype

Thematic Area(s): Scalable Computing Migration

PI Name: Dr. David Bernholdt (NPAC-Syracuse)

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Project Description: DMSO recently introduced a new integration framework for advanced simulation networking called High Level Architecture (HLA), based on the Run-Time Infrastructure (RTI) software bus model. RTI enables federations of real-time/time-stepped and logical-time/event-driven simulations/federates and it optimizes communication via event filtering and publisher/subscriber region/interest matching, supported by the Data Distribution Management (DDM) service.

Full and rapid DoD-wide transition to the HLA is strongly advocated by DMSO and facilitated by open public specifications of all HLA components, extensive nation-wide tutorial programs and prototype RTI implementations. In particular, early prototype codes for RTI F.0 ("familiarization" release) and RTI 1.0 subsets were released by DMSO to the DoD simulation community in spring/fall 1997. The complete RTI 1.0 implementation, including full DDM support is expected by the end of 1997.

Given the systematic shift of the DoD training, testing and wargaming activities from the physical to synthetic environments, and the ever increasing computational demands imposed on advanced modeling and simulation systems, high performance distributed computing support for HLA will likely play the crucial role in the DoD HPC Modernization Program. Based on NPAC expertise in Web/Commodity Software based HPCC, they are proposing a focused project within the PET program that will address a critical aspect of rapid deployment of high performance HLA systems: World-wide distributed RTI on top of Java/CORBA based Object Web and focused on Web based collaborative HLA training. The DIS to HLA transition process is rapid and, for some people often complex or/and confusing. DMSO provides significant help to the community in terms of high level tutorials and prototype RTI codes. Additional help, as proposed in this project, could be provided by an open, source level RTI subset implementation using Object Web/Commodity technologies such as CORBA and Java. Such RTI would be made broadly accessible both at the source code and runtime/collaborative simulation level, and integrated into the existing and forthcoming HLA training and tutorial suites.

NPAC is currently developing Java based Web Object Request Broker (WORB) server that will support HTTP and IIOP protocols and will act as a universal node of the HPcc (High Performance commodity computing) environment. Given that the RTI object bus model is strongly influenced by CORBA and that DMSO is in fact interacting with OMG towards proposing HLA as CORBA simulation facility/framework, an early Java/CORBA based RTI prototype seems to be a natural effort in the domain of interactive HLA training. The NPAC Object Web/WORB based RTI subset will support and integrate Web DIS (Java and VRML based) applications under development at the Naval Postgraduate School in Monterey, CA, as well as more traditional and substantial simulation codes such as ModSAF and perhaps also SPEEDES, TEMPO or IMPORT, currently at the planning stage as possible FMS training targets for NPAC PET activities at ARL.

By the end of this project, NPAC will deliver a prototype object web (CORBA) based RTI kernel (subset), capable of running a simple demonstration application to be developed locally. This will serve as a demonstration of the integration of DMSO and web technologies and provide a freely available tool. A follow-on project can further develop the system into a full FTI implementation, at which point it would be possible to run real RTI applications as a demonstration of this tool.

Benefits: This project will enhance the ability of the FMS community to make use of HPCC resources.

Deliverables: CORBA/HPCC based implementation of RTI kernel (subset) with simple application for demonstration purposes (March 1998)

Notes: Concurrently with this project, ARL will be supporting an analysis of DMSO RTI with regard to parallelization. Both projects should be completed by or before March 1998; then one can decide on zero, one, or both of:
ï   Implement Parallelization of DMSO RTI
ï   Complete Public Domain CORBA HPCC based RTI which should be able to run significant FMS applications

The relationship between these projects might be understood by analogy with MPI (RTI being a runtime infrastructure to support general event and time stepped simulations). There are a variety of different MPI implementations, both freely available and commercial. They have different target platforms (networks of workstations, MPPs, etc.), different performance, and different strengths. Similarly, the CORBA/HPCC RTI project shows the relationship with emerging distributed HPCC

commodity technologies, while the other focuses adapting DMSO RTI to work more efficiently on a large HPC platform.

NPAC emphasizes that FMS and HPCC are not easy to mix, as there has been little work in this area, and so up-front technology development is required. There are no obvious (to NPAC) HPCC FMS activities which can deliver real results very quickly. [Note: NPAC has extensively interacted with Dr. Robert Wasilausky and understands his needs. They are going to NRaD early November to continue this interaction. They understand that continued work with Wasilausky is essential and will continue to do this.]

The work NPAC proposes is not without risk as they are essentially addressing issues that have not been studied. NPAC believes these approaches are technically sound and this evaluation is based on their experience in both fields. They cannot give the same certainty in this work as, say porting MPI, would allow.

Customer Commitment/Involvement: The FMS CTA lead has requested parallelization of RTI and examination of web technologies in this context.

9. Title: 3-D ADCIRC Parallel Migration

Thematic Area(s): Scalable Computing Migration

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PI Telephone: (512) 475-8626   **PI Fax:**   (512) 471-8694

Project Description: Texas proposes to migrate the 3-D version of ADCIRC (Advanced
Circulation Model) to the parallel platforms at CEWES MSRC. This
effort will proceed in the following stages:

1) A parallel grid partitioning algorithm based on space-filling curves will
be developed to partition an unstructured grid among a user-specified
number of processors.

2) A pre-processor code will be developed using the grid partitioning
kernel to split global input files currently used in 3-D ADCIRC into local
input files for each processor.

3) The 3-D version of ADCIRC uses its own pre-processor to
comment/uncomment certain lines in the code depending on the
architecture (workstation, vector machine, etc.). Texas will extend this
preprocessing capability to include parallel machine-specific (i.e., MPI
calls). This step also includes placing appropriate MPI calls within the
code for message-passing between processors.

4) A post-processing code will be developed which converts local output
files generated by each processor into global output files for plotting and
data analysis.

5) For the ease of users, scripts and makefiles will be developed to
compile the above-mentioned codes using machine-specific compile
commands, and to execute the codes.

6) The codes will be tested and debugged in collaboration with CEWES
MSRC users. User's manuals will be written detailing the pre-processor,
post-processor, and parallelization of 3-D ADCIRC.

7) A training session with interested CEWES MSRC users on the parallel
code will be held.

The parallelization model to be followed is similar to the approach Texas
used to successfully parallelize CE-QUAL-ICM. However, Texas must

18

develop a more efficient grid-partitioning code which can handle the large datasets used in circulation modeling (30,000-1,000,000 elements).

Benefits: The 3-D version of ADCIRC has been identified as an essential element toward coupling EQM and CWO computational systems.

Deliverables:
15 Dec 97 -- Parallel grid partitioning code
1 Jan 98 -- Pre and post-processing codes and MPI calls in ADCIRC
Jan-Mar 98 -- Testing and debugging
15 Mar 98 -- User's manual written and training session scheduled

Customer Commitment/Involvement: This effort has the support of cognizant CEWES MSRC users, including Norm Scheffner, Rao Vemulakonda and Carl Cerco. Texas is also in close collaboration with the developers of ADCIRC, Rick Luettich and Johannes Westerink.

10. Title: Incorporation of PARSim into GMS

Thematic Area(s): Scalable Computing Migration

PI Name: Dr. Mary Wheeler (TICAM-Texas)

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Project Description: PARSim (Parallel Aquifer and Reservoir Simulator) is a 3-D flow and transport simulator for modeling contamination and remediation of soils and aquifers. It was developed at the University of Texas at Austin. The code uses sophisticated numerical methods for solving the flow and transport equations and includes very general reaction kinetics, including geochemical and biogeochemical processes. The code is fully parallelized using domain decomposition and MPI and is operational on the SP and T3E platforms. Texas proposes to incorporate PARSim into GMS (Groundwater Modeling System) and develop procedures required to "launch" PARSim on any of the parallel hosts at CEWES MSRC. This project is intended to provide a proof of concept for launching within the GMS framework.

Benefits: The GMS module runs on high-end workstations. There is a very strong desire on the part of EQM leadership to have capability to ìlaunchî HPC codes from this framework.

Deliverables:
1 Jan 98 -- Incorporate PARSim into GMS
1 Mar 98 -- Completion of an execution shell to automate launching procedures
28 Mar 98 -- Schedule training session to train CEWES MSRC users on launching process

Notes: None.

Customer Commitment/Involvement: This effort was specifically requested by Dr. Jeff Holland, DoD CTA Lead for EQM.